Phenomenological description of competing antiferromagnetism and d-wave superconductivity in high T_c cuprates

Bumsoo Kyung and A. M. -S. Tremblay[1]

Département de physique and
Centre de recherche sur les propriétés électroniques de matériaux avancés.
[1]*Institut canadien de recherches avancées*
Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

(April 23, 2002)

In this paper the phase diagram of high T_c cuprates is *qualitatively* studied in the context of competing orders: antiferromagnetism, d-wave superconductivity and d-density wave. *Local* correlation functions are estimated from a mean-field solution of the $t-J$ Hamiltonian. With decreasing doping the superconducting mean-field T_c^{MF} and order parameter d begin to decrease below some characteristic doping $x_c \simeq 0.2$ where short-range antiferromagnetic correlations begin to develop. *Dynamical* properties that involve the energy spectrum, such as the normal state pseudogap, are calculated from effective interactions that are consistent with the above-mentioned local correlation functions. The total excitation gap Δ_{tg} (in the superconducting state) and the normal state pseudogap Δ_{pg} are in good agreement with experimental results. Properties of the condensate are estimated using an effective pairing interaction V_{eff} which takes into account (pair breaking) antiferromagnetic correlations. These condensate properties include condensation energy $U(0)$, coherence gap Δ_{cg} and critical field H_{c2}. The calculated coherence gap closely follows the doping dependence of T_c or d, and is approximately given as $\Delta_{cg} \sim \Delta_{tg} - \Delta_{pg}$ within our numerical uncertainties. The systematic decrease of superfluidity (d, $U(0)$, Δ_{cg}, H_{c2}), and systematic increase of Δ_{pg} and Δ_{tg} with decreasing doping below x_c have their natural explanation in our approach. The overall description is however qualitative since it does not appear possible to obtain results that are in quantitative agreement with experiment for all physical quantities.

I. INTRODUCTION

Fifteen years have passed since the discovery of high temperature superconductivity in $Ln_{2-x}Ba_xCuO_4$ by Bednorz and Müller, [1] yet there is no widely accepted theoretical explanation of the many anomalous features found in these materials. This is due to a large extent to the lack of reliable theoretical methods to study this strongly-correlated electron problem. Dynamical Mean Field theory, for example, [2] works extremely well in three or higher dimensions but it lacks the momentum-dependent self-energy effects that are intrinsic to a two-dimensional situation with strong antiferromagnetic fluctuations. More recent dynamical cluster approaches correct this defect but these methods are still in their infancy and are entirely numerical. [3] [4] In this paper, we step back and take a more humble stand, seeking the *simplest phenomenological* approach that describes the main *overall* features of high-temperature superconductors. Let us recall what these features are.

First consider the generic phase diagram of a hole-doped cuprate $Ln_{2-x}Sr_xCuO_4$ in the doping ($x = 1 - n$) and temperature (T) plane. [5] Near half-filling and at low temperature, antiferromagnetic (AF) long-range order appears and is destroyed by 2% doping concentration ($x = 0.02$). When x reaches 0.05, superconducting (SC) long-range order starts to appear and is also destroyed by about 30% doping. In between them, T_c reaches a maximum value at $x \simeq 0.15$. The SC gap was found to have mainly d-wave character, [6–9] in contrast to conventional BCS superconductors [10] with an isotropic s-wave gap.

Second, various recent experiments also show the existence of a crossover temperature T^* higher than T_c in underdoped and optimally doped samples. Below this so-called pseudogap temperature T^*, low-frequency spectral weight begins to be strongly suppressed in many physical quantities. This anomalous phenomenon has been observed in angle resolved photoemission spectroscopy (ARPES), [11,12] specific heat, [13] tunneling, [14] NMR, [15] and optical conductivity. [16] Surprisingly the doping dependences of T^* and T_c are completely different [17,18] in spite of their possibly close relationship suggested by ARPES [11,12] and tunneling [14] experiments. At optimal doping, where T_c is maximum, various non-Fermi liquid (NFL) properties are observed in the normal state. These include the linear temperature dependence (up to $1000K$) of ab-plane resistivity, the quadratic T dependence of Hall angle and so on. Far beyond optimal doping, there are indications that the normal state properties are probably well described by the conventional Landau Fermi liquid. Near and below optimal doping, the superfluid density n_s/m is systematically suppressed

1

with decreasing doping in spite of the increasing excitation gap amplitude, as measured by ARPES, in the superconducting state. The resulting $2\Delta_{max}/k_B T_c$ ratio is very different from the universal BCS value, 4.3 for d-wave symmetry. In the overdoped regime, however, the SC properties are probably well explained in the conventional weak-coupling BCS theory, although this has not yet been checked in detail. [19]

The approach that we take is as follows. First, we do a simple mean-field analysis of the $t - J$ Hamiltonian whose results are used only to obtain estimates for zero-temperature order parameters and to compute equal-time local correlation functions (such as double occupancy). Dynamical quantities, such as the response functions and single-particle spectral weight, are computed by using the values of the local correlation functions obtained in mean field to fix the value of the renormalized interaction vertices. We do not consider the possibility of spin-charge separation [20,21] but we take into account the no-double-occupancy constraint by replacing projectors in the $t - J$ Hamiltonian by their mean-field bosonic value, namely doping x. This is an effective-mass approximation. We cannot address the issue of a quantum critical point (QCP) [22] at x_c even if it exists at the mean-field level. Non-Fermi liquid behavior above the pseudogap temperature is also beyond the domain of validity of our approach. The regime we consider is one where the temperature would normally be low enough for a Fermi liquid to appear but where fluctuations destroy that phase, especially in the underdoped regime.

The paper is organized as follows: In Section II the $t - J$ Hamiltonian is decoupled, in a mean-field approximation, with competing (SC, AF and $d-$density wave) order parameters. The mean-field Hamiltonian is diagonalized to compute mean-field ordering temperatures T_c^{MF}, T_N^{MF} and mean-field order parameters d and m. Dynamical quantities such as the normal-state pseudogap are computed and compared with experimental results in Section III. In Section IV the results of the previous sections are gathered to discuss the phase diagram of high T_c cuprates. In Section V we discuss some of the properties of the SC condensate, such as the condensation energy, upper critical magnetic field and the coherence gap, using a model that takes into account the effect of (pair breaking) AF correlations in an effective manner. The present results are compared with some of the leading theories for the high T_c superconductivity in Section VI as well as with experiments. The last Section summarizes the results and discusses its main limitation.

II. MEAN-FIELD $T - J$ HAMILTONIAN

Right after the discovery of high temperature superconductors, Anderson [23] first proposed the one-band Hubbard model as the simplest Hamiltonian that might capture the correct low energy physics of copper oxides. The $t - J$ model is known to be the large U limit of the Hubbard Hamiltonian under certain assumptions. The $t - J$ model is described by the Hamiltonian

$$
\begin{aligned}
H = & -t \sum_{\langle i,j \rangle, \sigma} \left((1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) + \text{H.c.} \right) \\
& + J \sum_{\langle i,j \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right) - \mu \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} ,
\end{aligned} \tag{1}
$$

where $c_{i,\sigma}$ destroys an electron at site i with spin σ on a two-dimensional square lattice, t is the hopping matrix element between nearest neighbors $< i, j >$ and J denotes superexchange coupling. Double occupancy of two electrons at the same lattice site is forbidden in the Hilbert space corresponding to Eq.(1) as can be seen by the projection operator $(1 - n_{i,-\sigma})$ in the hopping term. The chemical potential μ controls the electron density n. Finally, $\vec{S}_i$ and n_i are spin and charge density operators, respectively, and they are defined by

$$
\begin{aligned}
\vec{S}_i &= \frac{1}{2} \sum_{\alpha,\beta} c_{i,\alpha}^\dagger \vec{\sigma}_{\alpha,\beta} c_{i,\beta} , \\
n_i &= \sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma} ,
\end{aligned} \tag{2}
$$

where the components of $\vec{\sigma}$ are 2×2 spin Pauli matrices.

In general the (static) mean-field description is not accurate for strongly correlated electron systems such as the Hubbard and $t - J$ models in the physically relevant regime. Nevertheless it is known that, for example, the mean-field description of the antiferromagnetic state at $x = 0$ is quite accurate, even at large U. For example, spin waves with accurate spin-wave velocities can be obtained by performing RPA in the ordered phase. [24] We take the point of view that mean-field theory can be useful to select the leading correlations when there are several *competing* order parameters in the low energy sector. Due to the neglect of spatial and quantum fluctuations in mean-field theory, some caution is necessary in interpreting the results. First, the mean-field phase line is to be decreased in temperature to take into account the effect of quantum fluctuations (such as Kanamori-Brueckner screening [25]). Second, since we work in two dimensions where antiferromagnetic long-range order is prohibited by the Mermin-Wagner theorem, the renormalized mean-field Néel transition line has to be interpreted as the onset of the corresponding *short-range* correlations instead of as a *true* thermodynamic phase transition. Whether given short-range correlations eventually grow to long-range order at low temperature or not, should be answered by studying how the zero-frequency correlation length grows when temperature is lowered. This question, as well as that of dynamical or quantum fluctuations that may take place on very short distance

scales [2] can be examined by the fluctuation theory that we describe in Section III.

In the spirit of a mean-field approximation, terms with more than two operators should be decoupled in all possible ways. In principle there are infinitely many ways of decoupling the Heisenberg part of the Hamiltonian. In this situation, guidance from experiments and past theoretical considerations is helpful to find the most important leading correlations of the model, correlations whose stability is studied *a posteriori*. We consider three *competing* mean-field order parameters, m, d, and y for AF, d-wave SC, and d-density wave [26] orders respectively, which are defined [27] by

$$m = \langle \hat{m} \rangle = 1/(2N) \sum_{\vec{k},\sigma} \sigma \langle c^{\dagger}_{\vec{k}+\vec{Q},\sigma} c_{\vec{k},\sigma} \rangle, \tag{3}$$

$$d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} \phi_d(\vec{k}) \langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \rangle , \tag{4}$$

$$y = \langle \hat{y} \rangle = i/(2N) \sum_{\vec{k},\sigma} \phi_d(\vec{k}) \langle c^{\dagger}_{\vec{k}+\vec{Q},\sigma} c_{\vec{k},\sigma} \rangle, \tag{5}$$

where N is the total number of lattice sites, $\phi_d(\vec{k}) = \cos k_x - \cos k_y$ is the $d-wave$ form factor and $\vec{Q}$ is the (commensurate) AF wave vector (π, π) in two dimensions. The extended $s-$wave analogs of $d-$wave superconductivity and $d-$density wave orders are also present in the $t-J$ Hamiltonian, but they are always less relevant in mean-field studies. In this paper we restrict ourselves to a uniform solution. At the end of the paper the issue of inhomogeneous modulation of spin and charge degrees of freedom will be briefly discussed in the context of the present results. A similar mean-field decoupling for the AF and SC channels only was previously considered by several groups. [28,29] In the present study the projected operator $c_{j,\sigma}(1-n_{j,-\sigma})$ is separated into the original electron operator $c_{i,\sigma}$ times the expectation of the bosonic operator $(1 - n_{j,-\sigma})$ which is taken as $x^{1/2}$. As long as the no-double-occupancy constraint is *globally* imposed, the average number of electron n_e in our study is equal to $1 - n_h$ with $x = n_h$. Clearly, at half-filling, one recovers the Heisenberg Hamiltonian. In addition, as we shall see later, for $T = 0$, $n = 1$, the no-double-occupancy constraint is satisfied *exactly* because the AF solution allows only one electron per site with the full moment. This would not be the case if we considered only $d-$wave and $d-$ density wave mean-field solutions.

For a more systematic implementation of this constraint beyond the mean-field level, the slave boson representation can be useful. [30,31] In the slave boson representation, an electron is explicitly decomposed into a spinon (fermion) and a holon (boson), $c^+_{i,\sigma} = f^+_{i,\sigma} b_i$. The latter bosonic operator corresponds to $(1 - n_{i-\sigma})$ in our approach and our global constraint $1 = n_e + n_h$ corresponds to the no double-occupancy constraint in slave boson mean-field theories.

In terms of mean-field order parameters m, d, and y, the mean-field $t - J$ Hamiltonian reads

$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^{\dagger}) - Jy\hat{y} + F_0 ,$$
$$\tag{6}$$

where

$$F_0 = N(2Jm^2 + Jd^2 + \frac{J}{2}y^2 - \mu) . \tag{7}$$

$\varepsilon(\vec{k}) \simeq -2tx(\cos k_x + \cos k_y) - \mu$ with x the hole density. The correlated hopping is taken into account through x in a mean-field spirit, as explained above. In other words, the no-double-occupancy constraint manifests itself here as an effective mass, not as a change in the number of carriers. One has to keep in mind however that, at this level, $\varepsilon(\vec{k})$ and the corresponding effective mass are only bare values that are renormalized by interactions. This is discussed further at the end of the following section.

Previous studies have suggested that the $d-$density wave order parameter becomes important only quite close to half-filling. [32] Here we find that this order parameter is *never* a self-consistent solution of the mean-field equations when mean-field AF order is explicitly considered in Eq.(6). Hence, in the following, we restrict ourselves to AF and SC order parameters. By introducing a four component field operator $\Psi^{\dagger}_{\vec{k}}$

$$\Psi^{\dagger}_{\vec{k}} = (c^{\dagger}_{\vec{k},\uparrow}, c_{-\vec{k},\downarrow}, c^{\dagger}_{\vec{k}+\vec{Q},\uparrow}, c_{-\vec{k}-\vec{Q},\downarrow}) ,$$

Eq. (6) may be written in a more compact form to reflect the competition between AF and SC order,

$$H_{MF} = \sum_{\vec{k}}{}' \Psi^{\dagger}_{\vec{k}} M_{\vec{k}} \Psi_{\vec{k}} + F_0 .$$

The prime symbol on the summation restricts the summation over wave vectors to the magnetic Brillouin zone in order to take into account the doubling of the unit cell in the presence of (commensurate) AF order. Small incommensuration would not change appreciably the value of the local correlation functions that we will compute with the mean-field solution, hence we limit ourselves to the commensurate case. The matrix $M_{\vec{k}}$ in the last equation is given by

$$M_{\vec{k}} = \begin{pmatrix} \varepsilon(\vec{k}) & -Jd\phi_d(\vec{k}) & -2Jm & 0 \\ -Jd\phi_d(\vec{k}) & -\varepsilon(\vec{k}) & 0 & -2Jm \\ -2Jm & 0 & \varepsilon(\vec{k}+\vec{Q}) & Jd\phi_d(\vec{k}) \\ 0 & -2Jm & Jd\phi_d(\vec{k}) & -\varepsilon(\vec{k}+\vec{Q}) \end{pmatrix} . \tag{8}$$

The energy eigenvalues of $M_{\vec{k}}$ yield four branches to the energy dispersion $\pm E_{\pm}(\vec{k})$

3

$$E_\pm(\vec{k}) = [(\varepsilon_{\vec{k}}^2 + \varepsilon_{\vec{k}+\vec{Q}}^2)/2 + (2Jm)^2 + (Jd\phi_d(\vec{k}))^2$$
$$\pm g(\vec{k}) \ ]^{1/2} \ , \tag{9}$$

where $g(\vec{k})$ is given as

$$g(\vec{k}) = [(\varepsilon_{\vec{k}}^2 - \varepsilon_{\vec{k}+\vec{Q}}^2)^2/4 + ((\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{Q}})(2Jm))^2]^{1/2} \ . \tag{10}$$

The free energy is easily obtained either from the trace formula or from the Feynman theorem

$$F = -2T \sum_{\vec{k}}{}' \sum_{\alpha=\pm} \log(2\cosh\frac{E_\alpha(\vec{k})}{2T}) + F_0 \ .$$

Two mean-field equations are obtained from the stationary condition on F with respect to the corresponding order parameters, $\frac{\partial F}{\partial m} = \frac{\partial F}{\partial d} = 0$, and one more unknown constant μ is determined by the thermodynamic relation $n = 1 - x = -\frac{\partial F}{\partial \mu}$. The resulting three equations are

$$m = \frac{1}{2N}\sum_{\vec{k}}{}'\sum_{\alpha=\pm}\left\{(2Jm) + \alpha\frac{(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{Q}})^2(2Jm)}{2g(\vec{k})}\right\}$$
$$\times\frac{1}{E_\alpha(\vec{k})}\tanh(\frac{\beta E_\alpha(\vec{k})}{2}) \ ,$$

$$d = \frac{1}{2N}\sum_{\vec{k}}{}'\sum_{\alpha=\pm}\phi_d^2(\vec{k})(Jd)\frac{1}{E_\alpha(\vec{k})}\tanh(\frac{\beta E_\alpha(\vec{k})}{2}) \ ,$$

$$n = 1 - \frac{1}{2N}\sum_{\vec{k}}{}'\sum_{\alpha=\pm}\left\{(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{Q}})\right.$$
$$+\alpha\frac{(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{Q}})(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{Q}})^2}{2g(\vec{k})}$$
$$\left.+\alpha\frac{2(2Jm)^2(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{Q}})}{g(\vec{k})}\right\}\frac{1}{E_\alpha(\vec{k})}\tanh(\frac{\beta E_\alpha(\vec{k})}{2}) \ . \tag{11}$$

The spin-triplet order parameter $\langle c_{\vec{k}+\vec{Q},\uparrow}c_{-\vec{k},\downarrow}\rangle$ is "dynamically generated" [33] when the two mean-field order parameters m and d coexist, even when it is not explicitly included in the mean-field factorization. We have checked that including this order parameter in the mean-field factorization changes the value of local correlation functions, such as $\langle|\Delta_d(0)|^2\rangle$ which we need below for the dynamical calculation, by less than one percent. The values of m and d, on the other hand, change by about 10%. The inclusion of this order parameter would then change the results of the present paper only quantitatively and at the few percent level only. We do not include it for now for simplicity. It should be included at a later stage when refining the approach.

Even though it is only an intermediate step in our calculations, for completeness we show in Fig.1 the calculated mean-field phase diagram and zero-temperature
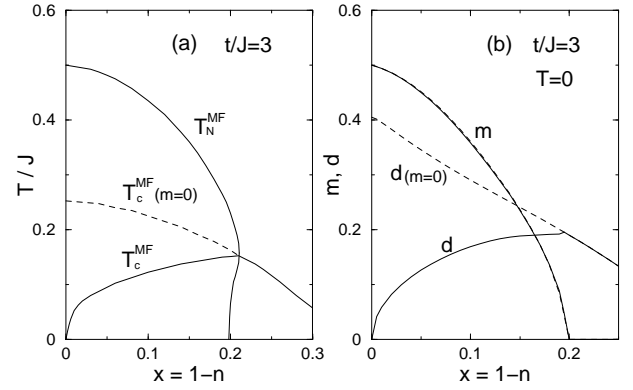

FIG. 1. (a) Calculated mean-field phase diagram in doping ($x = 1 - n$) and temperature (T) plane and (b) mean-field order parameters for $t/J = 3$. T_N^{MF} and T_c^{MF} are mean-field AF and SC ordering temperatures, while m and d are mean-field AF and SC order parameters. $T_N^{MF}(m = 0)$ and $d(m = 0)$ (dashed curves) are SC ordering temperature and order parameter, respectively, when the mean-field factorization of the interaction term (J) is in the SC channel only. The dashed curve for $T_N^{MF}(d = 0)$ is also shown in (b) but it is indistinguishible from the case where d takes its mean-field value.

mean-field order parameters m and d for $t/J = 3$. The AF order parameter dominates near half-filling and vanishes beyond $x = x_c \simeq 0.20$. On the other hand, d-wave SC correlations keep growing with decreasing doping down to $x_c \simeq 0.20$ where the AF order parameter is non-zero. Below x_c, we observe that T_c^{MF} and d begin to monotonically decrease with decreasing doping. The physical origin of this decrease of T_c^{MF} and d should be a combination of the effects of local moment formation and of the onset of AF correlations that break time-reversal symmetry, both of which lead to the destruction of the SC state. The importance of AF correlations in reducing T_c to the experimental value ($\sim 100K$) was recently pointed out by Weng. [34] In between half-filling and x_c, AF and SC orders coexist at the mean-field level. The overall features are similar to previous results [33] based on a phenomenological model in which SC and AF orders come from different interaction terms.

The dashed curves in Fig.1(a) and (b) are T_c^{MF} and d when the interaction piece of the Hamiltonian is decoupled only in the (spinon) pairing channel in the slave boson mean-field theory [35] or, equivalently, when m is forced to zero in the present approach. This shows that, by itself, the diverging effective mass is not enough to reduce T_c^{MF} and d to zero at half-filling. In the slave-boson theory, T_c^{MF} and d keep increasing with decreasing doping. T_c^{MF} is interpreted as pseudogap temperature T^* and the corresponding ground state is dubbed as the resonating valence bond (RVB) state. [23] In this theory, the true T_c is governed by the Bose-condensation temperature of holons, which scales as x. Then the maximum T_c occurs at very small doping concentration ($x < 0.05$).

More recent versions of this slave-boson mean-field theory seem to correct this defect [36].

In the present study, the behavior of the mean-field order parameters reflects the competition between AF and SC correlations. As can be seen in Fig.1, SC correlations are most significantly modified due to the presence of (pair breaking) AF correlations, while the latter are virtually unchanged by the former. When Eq. 6 is converted into an effective Hamiltonian where the competing order parameters are expressed in terms of operators we find

$$H = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} - 2J\hat{m}\hat{m} - J\hat{d}^{\dagger}\hat{d} - \frac{1}{2}J\widehat{y}\widehat{y}. \quad (12)$$

In this notation, it is clear that interactions that generate AF are stronger than those that generate SC by a factor of two and that the interactions that generate $d-$density wave order are even smaller. Note that to be able to make this comparison, the order parameters are normalized [27] such that the largest value that either one of them can take in a mean-field solution is near $1/2$ (when all other order parameters are forced to zero). In particular then, even if we drop the $d-$density wave, this mean-field $t-J$ Hamiltonian is not $SO(5)$ symmetric [37] since in that case, the $\hat{m}\hat{m}$ and $\hat{d}^{\dagger}\hat{d}$ terms would have the same coefficients, so as to form a five-dimensional super-spin vector. [38]

III. DYNAMICAL PROPERTIES : EXCITATION PSEUDOGAPS

In a previous study of the two-dimensional attractive Hubbard model [39] it was shown, by comparisons with Quantum Monte Carlo calculations, that the BCS mean-field ground state gave a good estimate (few percent) of double-occupancy in the normal state when the interaction strength satisfied $|U| \gtrsim 3t$ and when the temperature is reasonably low (T of order $0.5t$ or less). We expect this should remain true for correlation functions that are local in space and time. On the other hand, for dynamical quantities mean-field theory itself is clearly a bad estimate. Instead of a true antiferromagnetic gap as in Fig.1, we expect to have a pseudogap.

In Ref. [40], the procedure used to compute the pseudogap size Δ_{pg} was as follows. Let $\Delta_d(i)$ be defined by

$$\Delta_d(i) = \frac{1}{2} \sum_{\delta} g(\delta)(c_{i+\delta,\uparrow}c_{i,\downarrow} - c_{i+\delta,\downarrow}c_{i,\uparrow}),$$

where $g(\delta)$ is a d-wave form factor given, in real space representation, by $g(\delta) = 1/2$ for $\delta = (\pm 1, 0)$, $-1/2$ for $\delta = (0, \pm 1)$, and 0 otherwise. The d-wave symmetry spin-singlet local correlation function, $\langle|\Delta_d(0)|^2\rangle$, is computed from the ground state mean-field solution [40] but with only m different from zero. In other words, it
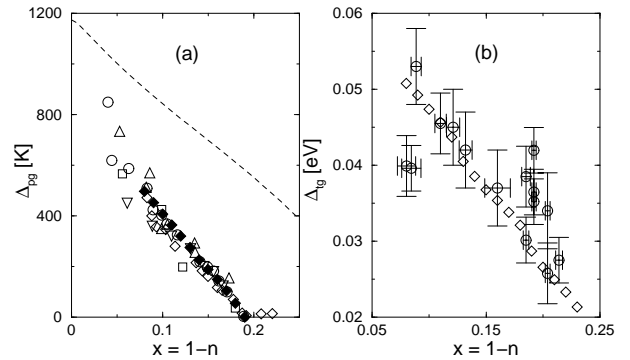

FIG. 2. (a) Calculated pseudogap size at $T = 0$, Δ_{pg}, denoted as filled diamonds for $t/J = 3.0$ and $J = 125$ meV. The open circles, diamonds, squares, up-triangles, and down-triangles are the pseudogap size extracted from susceptibility, heat capacity, ARPES, NMR, and resistivity measurements, respectively, by Tallon and Loram. [18] The dashed curve denotes (spinon) pseudogap size predicted by the slave boson mean-field theory of the $t - J$ model. (b) Calculated total excitation gap at $T = 0$, Δ_{tg} (empty diamonds). The empty circles with error bars denote ARPES leading edge gap by Ding *et al.* [43]

contains only AF correlations. This correlation function, $\langle|\Delta_d(0)|^2\rangle$, is then used in the fluctuation-dissipation theorem to obtain a renormalized vertex that allows one to estimate dynamical susceptibilities in any channel. [41] The latter come in the computation of both the two-particle and one-particle quantities. An example of such a calculation is given in section V. The pseudogap appears in the renormalized classical regime [42] of the singlet d-wave fluctuations in a region of the Fermi surface, namely the zone edges, where the thermal de Broglie wavelength is so small that it can become smaller than the d-wave zero-frequency correlation length even if the latter is of order only one lattice spacing. To be more specific, for $x = 0.1$ for example, the pseudogap appears near the zone edge when $T = 0.40J$. At this temperature, the characteristic energy of the $d-$wave singlet fluctuations is $0.31J$ while the corresponding correlation length estimated from the wave vector dependence of the $\omega = 0$ $d-$wave singlet susceptibility around $q = 0$ is 0.48 lattice spacing.

In Fig. 2(a) the calculated pseudogap size Δ_{pg} (filled diamonds) from Ref. [40] is plotted along with the pseudogap energy (empty symbols) extracted from various experiments by Tallon and Loram. [18] Note that the pseudogap rapidly takes its asymptotic low-temperature value when it opens up at finite temperature. That is the reason why we plot the value it would have at $T = 0$ if the superconducting phase did not appear. Since in the above calculational procedure, the local $d-$wave singlet correlation function $\langle|\Delta_d(0)|^2\rangle$ that is used to compute the dynamical singlet susceptibility is computed from static antiferromagnetic mean-field order, the corresponding nor-

mal state pseudogap Δ_{pg} vanishes at $x \simeq x_c$. The calculated Δ_{pg} is in good agreement with experimental results. [44] Through interlayer tunneling spectroscopy of $Bi_2Sr_2CaCu_2O_{8+\delta}$ Krasnov [45] also observed that the pseudogap decreases approximately linearly with doping and vanishes at the critical doping, $x_c \simeq 0.19$.

The dashed curve is the pseudogap size predicted from the slave-boson mean-field theory of the $t - J$ Hamiltonian. [35] In fact the (spinon) pseudogap size obtained in the latter theory is the same as $2Jd$ calculated from Eq.(6) with $m = 0$. It is much larger than the experimentally extracted pseudogap energy throughout the interesting doping range. Furthermore there is no indication that it vanishes near x_c, in conflict with experimental results. Although spin degrees of freedom are the main driving force for the pseudogap behavior in the above theory and in ours, the detailed implementation is qualitatively different. In the slave-boson mean-field theory a pseudogap is caused by a pairing among *spinons*, while in our theory it is *short-range* spin correlations of *electrons* that induce an effective attraction in the particle-particle channel. The spinon pseudogap in the former theory has nothing to do with local moment formation and their short-range AF correlations with decreasing temperature.

The total excitation gap Δ_{tg}, at $T = 0$, is obtained [40] by allowing both d and m to be different from zero in the calculation of the quantity $\langle|\Delta_d(0)|^2\rangle$ that is used in the fluctuation-dissipation theorem to obtain the renormalized vertices entering the calculation of dynamical quantities. The calculated total excitation gap (or ARPES leading edge gap or SC gap), Δ_{tg}, at $T = 0$ is also plotted in Fig. 2(b) as a function of doping with $t/J = 3$. The open circles with error bars are experimentally determined leading edge gap by Ding *et al.* [43] in their ARPES measurement. Except a few points, which may be due to the effect of impurities as noted by the authors, our calculated Δ_{tg} is in reasonable agreement with experimental results and decreases more or less linearly with doping. In addition, the velocity defined by

$$v_2 = \frac{\Delta_{tg}}{\sqrt{2}} \sin \frac{k_F}{\sqrt{2}}$$

ranges from 1.0 to $2.0 \times 10^6 cm/s$ when x varies from 0.2 to 0.1. Experiments on various compounds and dopings in that range give results of order $1.0 \times 10^6 cm/s$ according to Ref. [46] More recent ARPES results Bi-2212 [47] give a ratio of v_2/Δ_{tg} that can decrease by about a factor two from optimal to underdoping, while transport measurements suggest a much stronger doping dependence. [19] Note that in our calculations of Δ_{pg} and Δ_{tg} we use the experimentally determined value of exchange coupling $J = 125$ meV. The only adjustable parameter is the ratio t/J that we take, as in the previous sections, equal to 3.

Δ_{tg} is always larger than Δ_{pg} due to the additional contribution from $d \neq 0$ [40] to the local spin-singlet amplitude $\langle|\Delta_d(0)|^2\rangle$. Since the SC order parameter vanishes at T_c, the SC gap below T_c continuously evolves into the normal state pseudogap above T_c with the same momentum dependence and magnitude.

Finally we comment on the Fermi velocity in the nodal direction. [47] Tabulation of angle-resolved photoemission (ARPES) data for the Fermi velocity [46] along the zone diagonal in the range $0.1 < x < 0.15$ lead to Fermi velocities in the range range from 1 to $2.5 \times 10^7 cm/s$. However, recent ARPES data on LSCO [48] seem to suggest that the Fermi velocity along the diagonal is doping independent and of order $2.5 \times 10^7 cm/s$. A weak doping dependence for the limiting low frequency Fermi velocity is seen in Bi-2212. [49] Our *bare* Fermi velocity varies linearly with x, but to compare with ARPES experiment, one should include the effect of residual interactions. The superconducting d-wave part of the interaction does not renormalize the Fermi velocity along the nodal direction, but antiferromagnetic fluctuations do. For $x = 0.15$ and $T = 0.05J$, we find that the bare velocity, estimated from the dispersion of the spectral weight, renormalizes from $1.27aJ$ to 1.04 aJ. For $x = 0.1$, the peak in the spectral function is very broad and in fact the quasiparticle picture does not strictly applies since $\partial\Sigma/\partial\omega > 0$. Nevertheless, if we do like in experiment and measure the dispersion of the spectral weight maximum, we find that for T between [50] $0.2J$ and $0.1J$, the Fermi velocity renormalizes *up* (since $\partial\Sigma/\partial\omega > 0$)from 0.85 aJ to 0.95 ± 0.05 aJ. Hence, the physical value of the velocity is much more doping independent than the bare value suggests. Such doping-independent values were also found in variational calculations that take into account the no-double occupancy constraint. [51] For $t/J = 3$, and $J = 125meV$, our Fermi velocity in physical units is thus about $0.7 \times 10^7 cm/s$, which is smaller than experimental values by a factor 3 to 4.

IV. QUALITATIVE PHASE DIAGRAM OF HIGH T_C CUPRATES

Applying the fluctuation approach of the previous section with the effective theory of the next section, one can use the resulting dynamical SC susceptibility to estimate the value of the correlation length ξ_{sc} at the temperature where order appears according to mean-field theory. This length, ξ_{sc}, is of order one lattice spacing. We know that quantum renormalization effects (Kanamori-Brueckner type) should decrease even the mean-field T_c to a lower value $T_c^{'MF}$. In addition, thermal fluctuations decrease it even further. If we look empirically at the value of ξ_{sc} when one reaches the experimentally determined superconducting transition temperature T_c, one finds that at that temperature, $\xi_{sc} \simeq 3 - 4$. We know
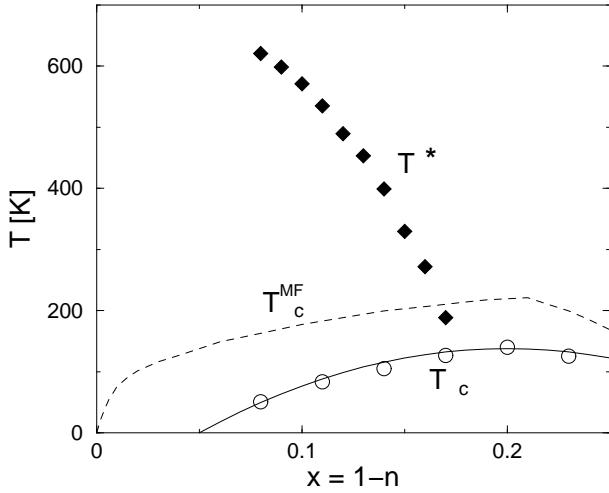
FIG. 3. Calculated phase diagram from fluctuation theory. T_c (empty circles) is the SC ordering temperature determined by fluctuation theory in which the correlation length ξ_{sc} becomes 4 lattice spacing. The solid curve is an interpolation of these points given as $T_c = -6122(x - 0.20)^2 + 138$ (K). T_c^{MF} (dashed curve) and T^* (filled diamonds) denote mean-field SC ordering temperature and pseudogap temperature, respectively.

that when the in-plane ξ_{sc} is sufficiently large, it should induce a three-dimensional SC transition. Since ξ_{sc} exponentially increases at low temperature in the renormalized classical regime, [25,39] the temperature where $\xi_{sc} \simeq 3 - 4$ is not much different from that where it is much larger. The empty circles in Fig. 3 are the value of T_c estimated from the above procedure ($\xi_{sc} = 4$). Unlike T_c^{MF}, T_c looks like a parabola centered at x_c. The solid curve is an interpolation formula for the data points given as $T_c = -4.22(x - 0.20)^2 + 0.095$ (units of J) or $T_c = -6122(x - 0.20)^2 + 138$ (K). In the same plot, the dashed curve is the mean-field SC temperature T_c^{MF} and the filled diamonds are the pseudogap temperature T^*. One expects that $O(2)$ SC fluctuations associated with superfluid stiffness should come into play only for $T_c'^{MF} \geq T \geq T_c$, as found by Corson *et al.* [52] in their terahertz spectroscopy measurements. This result contrasts with the SC fluctuation scenario for the pseudogap where SC fluctuations appear for $T^* \geq T \geq T_c$. The critical region for SC fluctuations appears larger at underdoping than at overdoping because of its small superfluid density. A rough estimate for the superfluid density is n/m^* which scales like $x(1 - x)$ in our approach because $n \sim (1 - x)$ and $1/m^* \sim x$. The pseudogap temperature T^* falls from a high value onto the T_c line [40] instead of sharing a common line with T_c in the overdoped region. This is because in our approach the d-wave singlet fluctuations that lead to the normal state pseudogap T^* are induced by short-range spin correlations. The latter *compete* in the low energy sector with SC correlations to make T_c go to zero near half-filling. [53] Note however

that since $O(2)$ SC fluctuations also cause a pseudogap close to T_c, [39] some experiments may suggest that the T^* line continues smoothly onto the dashed line (or more precisely the $T_c'^{MF}$ line) in the overdoped regime.

In the present study T_c and T_c^{MF} have their maximum at $x_c \simeq 0.20$ where condensation energy $U(0)$, mean-field order parameter d and the coherence gap Δ_{cg} discussed in the following section are also maximized. In high T_c cuprates, the highest T_c is at $x = 0.16$ slightly lower than the critical doping ($x = 0.19$) where the strength of superconductivity is maximum. [18] This subtle difference is beyond the scope of the present study.

Although short-range AF correlations persist up to x_c, they don't lead to long-range (commensurate) AF order, remaining only as short-range order even at low temperature, unless the electron density is close to half-filling. For instance, at $x = 0.15$, the AF correlation length ξ_{af} computed from fluctuation theory saturates at $\xi_{af} \sim 4$ at the lowest temperature studied while the SC correlation length ξ_{sc} exponentially diverges. Thus the long-range (commensurate) AF phase boundary is not shown in Fig. 3. It is expected to lie close to half-filling where the present formulation is not valid for AF spin fluctuations since the effective bandwidth, $8xt$ becomes smaller than interaction strength. [40]

V. THE CONDENSATE

At finite temperature algebraic (Kosterlitz-Thouless) superconducting order can develop in two dimensions, contrary to AF order, which is prohibited by the Mermin-Wagner theorem. Since short-range AF correlations can produce a (dynamical) pseudogap on short-distance scales while thermodynamic quantities, such as the SC condensate, are calculated in the static and long-distance limit, we should integrate out AF correlations to study the low energy physics of the SC state while taking into account the presence of the AF correlations in an effective manner. In principle, one should be able to do this and predict the onset of superconductivity from the interacting Green function of the previous sections, which exhibits a pseudogap. However, to do this calculation, one needs the corresponding irreducible vertex. It is not strictly correct to use the Thouless criterion in the form $1 - JGG = 0$ to find the superconducting T_c because one cannot use the bare vertex J to do a calculation with dressed Green functions. Since it is not known yet [25] how to obtain a reliable approximation for irreducible vertices in the pseudogap regime, we have to proceed otherwise. Calculations with constant renormalization to the vertices and bare Green functions are expected to be more reliable. The phenomenological correlation length criterion of the previous section is such a calculation.

We want to take into account the presence of short-range AF correlations. To proceed with a calculation
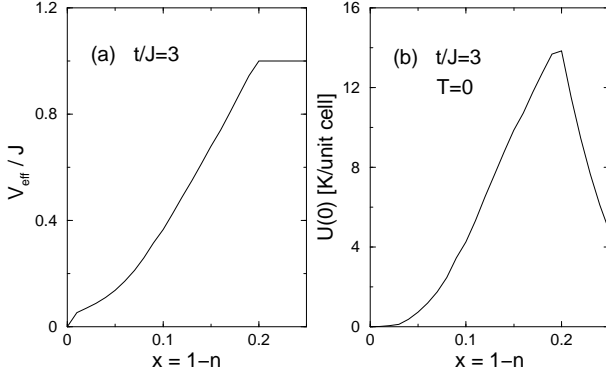
FIG. 4. (a) Effective strength of pairing interactions in the presence of (pair breaking) AF correlations and (b) calculated condensation energy at $T = 0$, as a function of doping concentration.

that is done with constant renormalization to the vertices and bare Green functions, we have to make an additional hypothesis. We construct an effective low-energy Hamiltonian

$$H_{eff} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} - V_{eff} \sum_i \Delta^+_d(i) \Delta_d(i) \quad (13)$$

such that the effective attraction V_{eff} leads, at $T = 0$, to the same value of the SC order parameter as that obtained from the full mean-field theory (Fig.1(b)). We will use this effective Hamiltonian only to compute properties of the condensate, including ξ_{sc} of the previous section. As long as superconductivity, or condensation, is concerned, the above Hamiltonian already takes into account the effect of (pair breaking) short-range AF correlations in an effective manner.

Above x_c, V_{eff} is given by J, because m vanishes there. We take the vanishing of m as signaling that the antiferromagnetic correlation length has become smaller than one lattice spacing. Below x_c, V_{eff} rapidly vanishes with decreasing doping in Fig.4(a). As a first application of the above effective Hamiltonian, let us calculate the condensation energy at $T = 0$. The total energies in the SC state and in the normal state are, in a mean-field approximation, given by

$$E_d = \langle \Psi_d | H_{eff} - \mu N | \Psi_d \rangle$$
$$= \sum_{\vec{k}} [(\varepsilon_{\vec{k}} - \mu) - \frac{(\varepsilon_{\vec{k}} - \mu)^2}{E_{\vec{k}}}] - |V_{eff}| d^2 ,$$
$$E_n = \langle \Psi_n | H_{eff} - \mu N | \Psi_n \rangle$$
$$= \sum_{\vec{k}} [(\varepsilon_{\vec{k}} - \mu) - |(\varepsilon_{\vec{k}} - \mu)|] , \quad (14)$$

where $E_{\vec{k}} = \sqrt{(\varepsilon_{\vec{k}} - \mu)^2 + (d\phi_d(\vec{k})V_{eff})^2}$. The $T = 0$ condensation energy $U(0) = -(E_d - E_n)$ is plotted in Fig. 4(b) as a function of doping concentration with $J = 125$ meV. $U(0)$ is maximum at x_c, and rapidly

decreases beyond and below x_c. This is because $U(0)$ scales like d^2. This feature is qualitatively consistent with specific-heat measurements by Loram et al. [54] The maximum $U(0)$ in our calculation is about $14K/$unit cell at x_c, two to three times larger than what the above authors obtained ($5 - 6K/$unit cell). It is clear that the actual condensation energy should be smaller than what we calculate since fluctuation effects are completely neglected in the above calculation. If we had stuck to a mean-field calculation with both AF and SC order present, we would have estimated the condensation energy from the difference between the ground-state energies computed with d finite and with d forced to zero. For $x > x_c$ we would have found the same result as on Fig. 4(b) and for $x < x_c$ we would have also found a result that decreases with doping, but it would have been larger than what is found above, suggesting that the above effective Hamiltonian approach is indeed a better way to take into account $T = 0$ long-range SC order in the presence of short-range AF correlations.

Another quantity of interest is the coherence-gap Δ_{cg}. Deutscher [55] has proposed that this gap, accessible through Andreev reflection experiments with point-contact spectroscopy, can be different from the single-particle gap observed in tunneling. Recent experiments [56] seem to confirm this. To estimate this coherence gap, one can use the mean-field solution of the effective BCS model Eq.(13). However, a better estimate can be obtained by computing the precursor pseudogap with the method explained below. Indeed, it is known [39] in the attractive Hubbard model that this precursor pseudogap reaches its asymptotic low-temperature value very rapidly. In addition, this precursor pseudogap contains quantum renormalization effects that are absent from a pure mean-field calculation. The following calculation is in the spirit of Ref. [40]. First we compute how much the d-wave pair correlation function χ_{pp} is enhanced over χ^0_{pp} by applying the local-pair sum rule for χ_{pp}

$$\frac{T}{N} \sum_q \chi_{pp}(q) e^{-i\nu_m 0^-} = \langle |\Delta_d(0)|^2 \rangle . \quad (15)$$

The right-hand side of the above equation is evaluated in the mean-field state of Eq. 13 and χ_{pp} is related to χ^0_{pp} through the renormalized vertex V_{pp}

$$\chi_{pp}(q) = \frac{\chi^0_{pp}(q)}{1 - V_{pp}\chi^0_{pp}(q)} ,$$

where the irreducible susceptibility is defined as

$$\chi^0_{pp}(q) = \frac{T}{4N} \sum_k (\phi_d(\vec{k}) + \phi_d(\vec{q} - \vec{k}))^2 G^0(q - k) G^0(k) .$$

Finally the following self-energy is used to estimate the effect of d-wave pairing correlations on quasiparticles.
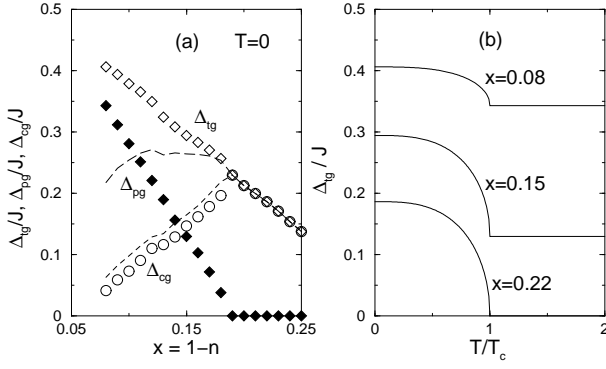
FIG. 5. (a) Calculated total excitation gap Δ_{tg} (empty diamonds), pseudogap Δ_{pg} (filled diamonds) and condensation gap Δ_{cg} (empty circles) at $T = 0$ as a function of doping. The dashed and long-dashed curves denote $\Delta_{tg} - \Delta_{pg}$ and $\sqrt{\Delta_{tg}^2 - \Delta_{pg}^2}$, respectively. (b) The total excitation gap Δ_{tg} as a function of temperature for three representative doping levels ($x = 0.08$ for underdoping, $x = 0.15$ for optimal doping and $x = 0.22$ for overdoping).

$$\Sigma_{pp}(k) = -\frac{1}{4} V_{eff} V_{pp} \frac{T}{N} \sum_q$$
$$(\phi_d(\vec{k}) + \phi_d(\vec{q} - \vec{k}))^2 \chi_{pp}(q) G^0(q - k) . \quad (16)$$

This procedure is analogous to that used earlier in the case of the attractive Hubbard model (s-wave symmetry) [39] to obtain good agreement with QMC calculations. Even though the above formula has not been obtained with the same rigor, one expects it to give a good estimate of what happens in the case of d-wave symmetry.

Figure 5(a) shows Δ_{cg} (empty circles) together with Δ_{tg} (empty diamonds) and Δ_{pg} (filled diamonds) as a function of doping at $T = 0$. Below x_c, Δ_{cg} monotonically increases with doping and above x_c it reduces to Δ_{tg}. The doping dependence of Δ_{cg} is qualitatively similar to T_c^{MF} and d, as found in the experiments of Ref. [56]. It is surprising to observe that Δ_{cg}, Δ_{tg} and Δ_{pg} are more or less linear in doping concentration, in spite of the fact that they are obtained through highly nonlinear equations. In fact the linear behavior of Δ_{tg} and Δ_{pg} in doping are observed by Tallon and Loram [18], and by Ding et $al.$ [43] in their respective experiments. To find out an empirical relation between Δ_{cg}, Δ_{tg} and Δ_{pg}, we plotted $\sqrt{\Delta_{tg}^2 - \Delta_{pg}^2}$ (long-dashed curve) and $\Delta_{tg} - \Delta_{pg}$ (dashed curve). The former is nearly independent of doping, in agreement with the result often found by other authors using $\Delta_{cg} = \sqrt{\Delta_{tg}^2 - \Delta_{pg}^2}$ [57] to extract the coherence gap from experiment. Within our numerical uncertainties, the coherence-gap Δ_{cg} is approximately given as $\Delta_{tg} - \Delta_{pg}$ and its behavior is easier to reconcile with the doping dependence of T_c and d. Recently Krasnov [45] also found that the coherence gap (dubbed as the SC gap in his paper) shows a doping dependence similar to that of T_c.

When $\Delta_{tg} \simeq \Delta_{pg} + \Delta_{cg}$ is generalized to finite temperature, the total excitation gap is composed of the normal state pseudogap and the coherence-gap in Fig.5(b). Δ_{pg} is virtually temperature independent from T^* to $T = 0$, because it is caused by short-range spin correlations of order one lattice spacing. On the other hand, we expect that Δ_{cg} is strongly temperature dependent since it opens up at T_c. For purposes of illustration, we added a BCS-like temperature dependence to Δ_{cg}. Its zero temperature-value and T_c were estimated above. As one can see from 5(b), at large underdoping ($x = 0.08$) Δ_{tg} (or ARPES leading edge gap) is mainly given by Δ_{pg}, while at optimal doping ($x = 0.15$) it is more or less equally made of Δ_{pg} and Δ_{cg} below T_c. At large overdoping ($x = 0.22$) $\Delta_{tg} = \Delta_{cg}$, thus leading to the conventional BCS behavior. This feature is also qualitatively consistent with ARPES experiments. [11,12]

A similar behavior of Δ_{tg} is used by Chen et $al.$ [57] to calculate the temperature dependence of some physical quantities within their SC fluctuation theory of the pseudogap. The crucial difference between their theory and ours is that their Δ_{pg} vanishes at $T = 0$ so that when superconductivity is completely destroyed, for instance, by a strong magnetic field, their ground state becomes a perfect Fermi liquid. In our picture, however, we predict that the ground state has a pseudogap. [40] Our calculated temperature dependence of the total excitation gap (or ARPES leading edge gap from the experimental point of view) contrasts with some theories based on the idea of spin-charge separation. In these theories the only difference between $A(\vec{k}, \omega)$ above and below T_c is the line shape due to the Bose condensation of holons, namely, the appearance of the quasiparticle peak below T_c without change of the gap magnitude itself. At large underdoping, there is indeed not much change in the ARPES leading edge gap [11,12], because from our point of view, Δ_{tg} is composed mainly of the temperature independent Δ_{pg}. At optimal doping the above ARPES experiments show a significant change of the excitation gap itself with decreasing temperature in addition to the sharpening of the peak. From our point of view, this significant change of Δ_{tg} (at optimal doping) with temperature is due to the strong temperature dependence of the coherence gap Δ_{cg} near the transition.

Since the zero-temperature critical field H_{c2} is a property of the condensate, the above V_{eff} model can also be used to estimate it. Using the d-wave estimate [58] $H_{c2} = 0.521 \Phi_0 \left(2\pi \xi_0^2\right)^{-1}$ with $\xi_0 = \hbar v_F \left(\pi \Delta_{cg}\right)^{-1}$ and $\Phi_0 = hc \left(2e\right)^{-1}$, we find that $H_{c2} (x = 0.08) = 42T$ and $H_{c2} (x = 0.15) = 151T$. The experimental values [59] are, respectively, around $30T$ and $60T$, somewhat smaller. However, there is still disagreement on the experimental value of H_{c2} and recent estimates are larger [60]. The above model is extremely crude since it does not take into account the anisotropy and interaction renormaliza-

tion of the Fermi velocity. Within this crude model, we have that H_{c2} will decrease at dopings larger than optimal because above optimal doping Δ_{cg} decreases.

VI. DISCUSSION

In this Section we compare the present results with the predictions of some of the leading theories for the high T_c superconductors and we provide further comparison with experiments. Before we proceed, we should stress that the starting point of our approach is meant to apply to the intermediate to strong-coupling regime and thus should be distinguished from spin-fluctuations theories that apply from weak to intermediate coupling. [61,62]

First, consider the question of why the superconducting T_c decreases near half-filling. As is clear by now, in our study the reduction of T_c near half-filling occurs already *at mean-field level* due to the competition with AF correlations (or local moment formation) that open up a mean-field gap, making SC order less favorable. Although SC fluctuations will indeed make T_c decrease with decreasing doping because of the smaller superfluid density [63,57], such fluctuations are not necessary to have the correct qualitative behavior.

Second, what is the nature of the normal state pseudogap? In this paper the pseudogap is just a crossover phenomenon due to short-range *equal-time* spin correlations which induce short-range *dynamical* fluctuations in the particle-particle channel. The latter are very effective in creating a pseudogap for several reasons. First note that the mass renormalization makes the bandwidth and the Fermi velocity quite small. In addition, the pseudogap opens up near the band edges where the local Fermi velocity is smallest. This means that the correlation length associated with the fluctuations does not need to be large to be in the renormalized classical regime. Second, for $q = 0$ d-wave singlet fluctuations, no umklapp condition needs to be satisfied contrary to antiferromagnetic hot spots. [64] The proposed origin for the pseudogap contrasts with some of the recent proposals in which *mean-field* flux phase, [65] circulating current phase, [66] and *d*-density wave phase [26] are interpreted as the pseudogap state. In these scenarios, the pseudogap state has broken symmetry such as time reversal, translational and rotational symmetries, and the crossover-like behavior observed in experiments is argued to be caused by an impurity effect.

Third, let us consider experimental evidence that there are significant short-range AF correlations below x_c. Recent muon spin relaxation [67,68] and ac-susceptibility measurements, show the existence of slow spin fluctuations below $x = 0.19$. By using polarized and unpolarized elastic neutron scattering experiments as well as zero-field muon spin resonance, Sidis *et al.* [69] observed an unusual commensurate AF phase on a nanosecond time

TABLE I. Temperature dependent antiferromagnetic correlation length evaluated for two dopings using fluctuation theory. The fluctuations may either be commensurate (C) or incommensurate (IC). The mesh used in the calculation was 128×128 hence the largest number in this table is a rough estimate.

	$x = 0.1$	$x = 0.15$
$T = 0.02J$	133 (IC)	4.1 (IC)
$T = 0.04J$	25.5 (C)	2.6 (IC)
$T = 0.06J$	6.1 (C)	1.9 (IC)

scale that coexists with superconductivity in underdoped $YBa_2Cu_3O_{6.5}$. Lake *et al.* [70] found AF correlations inside a vortex core in underdoped cuprates. Most recently, Hodges *et al.* [71] have even shown that the addition of Co to an optimally doped $YBCO$ compound induces antiferromagnetism above T_c that survives and coexists with $d - wave$ superconductivity below T_c. The coexistence seems to be at the microscopic level with $\xi > 200$Å. In the present paper, the presence of AF correlations below x_c does not come from any *extra* symmetry between AF and SC correlations such as $SO(5)$ symmetry, but from the fact that the J part of the $t - J$ Hamiltonian has those competing correlations in the low energy sector. Table 1 gives a few results for the temperature-dependent antiferromagnetic correlation length in our approach for two dopings. As expected, the correlations decrease with doping. An upper bound, order of magnitude estimate for the value of the static local moment is given by the value of m in Fig.1(b)

Fourth, we point out that there is numerical and experimental evidence that short-range spin correlations are closely related to the normal state pseudogap. In their recent calculations obtained from the *dynamical* cluster approximation (DCA) for the Hubbard model, Jarrell *et al.* [3] noted that the fall of T^* with doping is closely tied to the diminishing of the short-range spin correlations. In the exact diagonalization study of the $t - J$ model, Sakai and Takahashi [72] found that the pseudogap behavior is associated with the development of static AF spin correlations with decreasing temperature. In his high temperature series expansion study of the $t - J$ model, Putikka [73] showed that pseudogap crossover occurs when static AF correlation length is about one lattice spacing. By analyzing various experiments (Raman, spin-lattice relaxation rate, ARPES, Zn-substitution effects, inelastic neutron scattering experiment and so on), Tallon and Loram [18] concluded that the pseudogap is intimately connected with short-range AF correlations. Short-range dynamical AF correlations can also cause the normal state pseudogap through AF spin fluctuations. As explained above however, it was found in a recent paper [40] that the pseudogap always appears earlier in the dynamical particle-particle channel than in the dynamical AF spin fluctuation channel, even though the

short-range equal-time correlations that generate these dynamical fluctuations are due to AF correlations. One of the difficulties with AF spin fluctuation scenario of the pseudogap is how the normal state pseudogap happens to have the same momentum dependence and magnitude as the SC gap near T_c, [74] as ARPES and tunneling experiments show. In our case, this occurs naturally. Our results remain qualitatively the same when t' is $-0.3t$.

Fifth, is $x_c \simeq 0.19 - 0.20$ accidental for the special choice of $t/J = 3$? According to the calculations of the slave-boson mean-field solution of the Hubbard model [75,76], the onset of short range AF correlations starts to appear from $x = 0.20 - 0.21$ for a wide range of $U = 7t - 16t$ (See Fig.1 of Ref. [76] for more details). In our approach, x_c varies from 0.22 to 0.17 when t/J varies from 2.5 to 4. It is believed that a realistic strength of the Coulomb repulsion $U = 4t/J$ is of the order of the bare bandwidth $8t$ in two dimension. [77]

Last, through the microscopic separation of hole-rich SC regions from AF regions, [78] the stripe structure tends to maintain AF correlations more effectively than the other case in which they are uniformly suppressed by doped holes. Then one can surmise that in the stripe state T_c is somewhat suppressed from that in the uniform state. While the differences between the stripe state and the uniform state can be quite substantial, we do not see the stripes as necessary to obtain superconductivity. The main results reached in this paper are not expected to qualitatively change in the presence of a dynamical stripe structure.

VII. CONCLUSION

In this paper we proposed a simple phenomenological procedure that allows one to study the competition between antiferromagnetism and d-wave superconductivity in the high T_c cuprates. The no-double-occupancy constraint is taken into account in the effective mass approximation. Correlation functions that are local in space and time are evaluated from a mean-field factorization of the $t - J$ Hamiltonian in both the AF and the $d-$wave SC channels. (The $d-$density wave channel does not contribute in the whole doping range.) The local correlation functions are then used in the fluctuation-dissipation theorem to compute renormalized vertices that allow one to obtain the full *dynamical* susceptibilities. In other words, in this approach, equal-time correlation functions determine the value of effective vertices in all available channels. In particular, short-range equal-time AF correlations determine the value of effective interactions in the particle-particle channel. This effective weak to intermediate-coupling approach cannot work for $x < 0.08$ where the bandwidth becomes less than the interaction strength.

The calculated total excitation gap Δ_{tg} (in the superconducting state) and the normal state pseudogap Δ_{pg} are in good agreement with experimental results, as shown earlier in Ref. [40]. Obtaining a description of superconducting properties arising from a highly correlated state remains a challenge. Here we have taken the simplest approach. We compute an effective strength of pairing interactions which takes into account (pair breaking) AF correlations, V_{eff}, by requiring that the zero-temperature order parameter d obtained with V_{eff} equals that obtained in the full mean field equations corresponding to Eq.(6). This effective interaction allows one to obtain properties of the condensate (and of the condensate only), namely the condensation energy $U(0)$, the coherence gap Δ_{cg} that has been observed in Andreev reflection [56] as well as H_{c2}. The calculated coherence gap closely follows the doping dependence of T_c or d, and is approximately given as $\Delta_{cg} \sim \Delta_{tg} - \Delta_{pg}$ within our numerical uncertainties. A *qualitative* phase diagram for the cuprates may thus be obtained. The systematic decrease of $U(0)$, Δ_{cg} and H_{c2} with decreasing doping below $x_c \sim 0.2$ can be understood as a result of the competition between AF and SC order occurring in the low energy sector of the mean-field $t - J$ Hamiltonian. On the other hand, in the present picture the systematic increase of Δ_{pg} and Δ_{tg} when x decreases below $x_c \sim 0.2$ is due to the growing short-range *equal-time* spin correlations which induce *dynamical* singlet fluctuations with d-wave symmetry, low characteristic frequency but with small correlation length. As pointed out before in Ref. [40] one prediction of this approach is that the pseudogap should survive if the superconducting state is destroyed by a magnetic field. This is consistent with the observation of antiferromagnetic ordering inside vortex cores. [70] Neutron scattering experiments should be able to check from energy integrated structure factor that the short-range spin correlation functions are in good agreement with the mean-field predictions. Finally, we expect H_{c2} to decrease with doping in the overdoped region.

Although some of the results of this paper are in quantitative agreement with experiment, the overall description is definitely qualitative only. The main disagreement with experiment is that the *renormalized* Fermi velocity that we find is three to four times smaller than measured. A satisfactory theory of high T_c will necessitate a better treatment of strong-coupling short-range correlations.

[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).

[2] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

[3] M. Jarrell, Th. Maier, M. H. Hettler, and A. N. Tahvildarzadeh, cond-mat/0011282; Th. A. Maier and M. Jarrell, Phys. Rev. B **65**, 041104 (2002).

[4] Giulio Biroli, Gabriel Kotliar, cond-mat/0107108; Gabriel Kotliar, Sergej Y. Savrasov, and Gunnar Palsson, cond-mat/0010328.

[5] C. Almasan and M. B. Maple in *Chemistry of High Temperature Superconductors*, edited by C. N. R. Rao (World Scientific, Singapore, 1991).

[6] W. N. Hardy, D. A. Bonn, D. C. Morgan, R. Liang, and K. Zhang, Phys. Rev. Lett. **70**, 3999 (1993).

[7] B. G. Levi, Phys. Today, **46**, 17 (1993); *ibid.* **49**, 19 (1996).

[8] Z.-X. Shen, D. S. Dessau, B. O. Wells, D. M. King, W. E. Spicer, A. J. Arko, D. Marshall, L. W. Lombardo, A. Kapitulnik, P. Dickinson, S. Doniach, J. DiCarlo, T. Loeser, and C. H. Park, Phys. Rev. Lett. **70**, 1553 (1993).

[9] D. S. Marshall, D. S. Dessau, A. G. Loeser, C-H. Park, A. Y. Matsuura, J. N. Eckstein, I. Bozovic, P. Fournier, A. Kapitulnik, W. E. Spicer, and Z.-X. Shen, Phys. Rev. Lett. **76**, 4841 (1996).

[10] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[11] H. Ding, T. Yokoya, J. C. Campuzano, T. Takahashi, M. Randeria, M. R. Norman, T. Mochiku, K. Kadowaki, and J. Giapintzakis, Nature **382**, 51 (1996).

[12] A. G. Loeser, Z. -X. Shen, D. S. Dessau, D. S. Marshall, C. H. Park, P. Fournier, A. Kapitulnik, Science **273**, 325 (1996).

[13] J. W. Loram, K. A. Mirza, J. R. Cooper, and W. Y. Liang, Phys. Rev. Lett. **71**, 1740 (1993).

[14] Ch. Renner, B. Revaz, J. -Y. Genoud, K. Kadowaki, and ØFischer, Phys. Rev. Lett. **80**, 149 (1998).

[15] M. Takigawa, P. C. Hammel, R. H. Heffner, and Z. Fisk, Phys. Rev. B **43**, 247 (1991).

[16] C. C. Homes and T. Timusk, R. Liang, D. A. Bonn, and W. N. Hardy, Phys. Rev. Lett. **71**, 1645 (1993).

[17] T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999).

[18] J. L. Tallon and J. W. Loram, Physica C, **349**, 53 (2001); C. Bernhard, J. L. Tallon, T. Blasius, A. Golnik, and C. Niedermayer, cond-mat/0006288.

[19] Louis Taillefer, private communication.

[20] P. W. Anderson, Science **288**, 480 (2000).

[21] T. Senthil and M. P. A. Fisher, Phys. Rev. B **62**, 7850 (2000).

[22] S. Sachdev, *Quantum Phase Transitions*, Cambridge University Press, Cambridge (1999).

[23] P. W. Anderson, Science **235**, 1196 (1987).

[24] J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11663 (1989); Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996).

[25] Y. Vilk and A. M. Tremblay, J. Phys. I (France) **7**, 1309 (1997); S. Moukouri, S. Allen, F. Lemay, B. Kyung, D. Poulin, Y. M. Vilk, and A. M. S. Tremblay, Phys. Rev. B **61**, 7887 (2000).

[26] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001).

[27] Note that our definition of y differs by a factor $1/2$ from the original definition [26].

[28] M. Inui, S. Doniach, P. J. Hirschfeld, and A. E. Ruckenstein, Phys. Rev. B **37**, 2320 (1988).

[29] M. Inaba, H. Matsukawa, M. Saitoh, and H. Fukuyama, Physica C **257**, 299 (1996); J. Mizia, G. Gorski and K. Kucab, Phys. Stat. Sol. (b) vol.**229**, 1221 (2002).

[30] D. H. Lee, Phys. Rev. Lett. **84**, 2694 (2000).

[31] C. Nayak, Phys. Rev. Lett. **85**, 178 (2000).

[32] M.U. Ubbens, and P.A. Lee, Phys. Rev. B **46**, 8434 (1992).

[33] B. Kyung, Phys. Rev. B **62**, 9083 (2000).

[34] Z. Y. Weng, "High temperature superconductivity", edited by S. E. Barnes, et al., AIP conference proceedings 483, Woodbury, New York (1999) and cond-mat/9902124.

[35] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **69**, 973 (1987); P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987); G. Kotliar and J. Liu, Phys. Rev. B **38**, 5142 (1988); Y. Suzumura, Y. Hasegawa, and H. Fukuyama, J. Phys. Soc. Jpn. **57**, 401 (1988); Y. Suzumura, Y. Hasegawa, and H. Fukuyama, J. Phys. Soc. Jpn. **57**, 2768 (1988).

[36] J. Brinckmann and P. A. Lee, Phys. Rev. B **65**, 014502 (2002).

[37] S. C. Zhang, Science, **275**, 1089 (1997); S. Rabello, H. Kohno, E. Demler, and S. C. Zhang, Phys. Rev. Lett. **80**, 3586 (1998); C. L. Henley, Phys. Rev. Lett. **80**, 3590 (1998).

[38] Our definitions of AF and SC order parameters are equivalent to those appearing in SO(5) theory.

[39] B. Kyung, S. Allen, and A.-M. S. Tremblay, Phys. Rev. B. **64**, 075116 (2001).

[40] Bumsoo Kyung, Phys. Rev. B. **64**, 104512 (2001).

[41] Our approach is invalid for $x < 0.08$ because $8tx < 2J$ in that doping range, invalidating the weak coupling approach used in the calculation of dynamical quantities. For x larger than about 0.4, both zero temperature mean-field order parameters vanish meaning that correlations become more subtle. There is also no reason to believe that the effective-mass approximation is valid far from half-filling.

[42] Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).

[43] H. Ding, J. R. Engelbrecht, Z. Wang, J. C. Campuzano, S. -C. Wang, H. -B. Yang, R. Rogan, T. Takahashi, K. Kadowaki, and D. G. Hinks, cond-mat/0006143.

[44] This good agreement is in part fortuitous considering the various approximations used in this work. These include replacing the no-double-occupancy projector by x, eval-

uating local correlation functions in the mean-field state.

[45] V. M. Krasnov, Phys. Rev. B **65**, 140504 (2002).

[46] Qijin Chen, University of Chicago PhD thesis, 2000 (unpublished), p.97.

[47] J. Mesot, M. R. Norman, H. Ding, M. Randeria, J. C. Campuzano, A. Paramekanti, H. M. Fretwell, A. Kaminski, T. Takeuchi, T. Yokoya, T. Sato, T. Takahashi, T. Mochiku, and K. Kadowaki, Phys. Rev. Lett. **83**, 840 (1999).

[48] A. Lanzara, P. V. Bogdanov, X. J. Zhou, S. A. Kellar, D. L. Feng, E. D. Lu, T. Yoshida, H. Eisaki, A. Fujimori, K. Kishio, J. -I. Shimoyama, T. Noda, S. Uchida, Z. Hussain, and Z.-X. Shen, Nature **412**, 510 (2001).

[49] P. D. Johnson, T. Valla, A.V. Fedorov, Z. Yusof, B. O. Wells, Q. Li, A. R. Moodenbaugh, G. D. Gu, N. Koshizuka, C. Kendziora, Sha Jian, and D. G. Hinks, Phys. Rev. Lett. **87**, 177007-1 (2001).

[50] For $T = 0.05$ an antiferromagnetically-induced pseudogap opens up.

[51] Arun Paramekanti, Mohit Randeria, and Nandini Trivedi, Phys. Rev. Lett. **87**, 217002-1 (2001).

[52] J. Corson, R. Mallozzi, J. Orenstein, J. N. Eckstein, and I. Bozovic, Nature **398**, 221 (1999).

[53] S. Onoda and M. Imada, J. Phys. Soc. Jpn. Suppl. B **69**, 32 (2000).

[54] J. W. Loram, K. A. Mirza, J. R. Cooper, and J. L. Tallon, Physica C **282-287**, 1405 (1997); J. W. Loram, J. Luo, J. R. Cooper, W. Y. Liang, and J. L. Tallon, J. Phys. Chem. Solids **62**, 59 (2001).

[55] G. Deutscher, Nature **397**, 410 (1999); Y. Dagan, A. Kohen, G. Deutscher and A. Revcolevschi, Phys. Rev. B **61**, 7012 (2000).

[56] R.S. Gonnelli, A. Calzolari, D. Daghero, L. Natale, G.A. Ummarino, V.A. Stepanov, and M. Ferretti, cond-mat/0107289.

[57] Q. Chen, I. Kosztin, B. Janko, and K. Levin, Phys. Rev. Lett. **81**, 4708 (1998); Q. Chen, K. Levin, and I. Kosztin, Phys. Rev. B **63**, 184519 (2001).

[58] Wonkee Kim, Jian-Xin Zhu, and C.S. Ting, Phys. Rev. B **58**, R607 (1998).

[59] Yoichi Ando, G. S. Boebinger, A. Passner, L. F. Schneemeyer, T. Kimura, M. Okuya, S. Watauchi, J. Shimoyama, K. Kishio, K. Tamasaku, N. Ichikawa, and S. Uchida, Phys. Rev. B **60**, 12475 (1999).

[60] J. L. Luo, J. W. Loram, T. Xiang, J. R. Cooper, and J. L. Tallon, cond-mat/0112065.

[61] Andrey V. Chubukov, David Pines, and Jorg Schmalian, cond-mat/0201140.

[62] B. Kyung, Jean-Sébastien Landry, and A. -M. S. Tremblay, unpublished.

[63] V. J. Emery and S. A. Kivelson, Nature **374**, 434 (1995); M. Franz and A. J. Millis, Phys. Rev. B **58**, 14 572 (1998); M. Capezzali and H. Beck, Phsica B **259-261**, 501 (1998); H. J. Kwon and A. T. Dorsey, Phys. Rev. B **59**, 6438 (1999).

[64] Y. M. Vilk, Phys. Rev. B **55**, 3870 (1997).

[65] X. -G. Wen and P. A. Lee, Phys. Rev. Lett. **76**, 503 (1996).

[66] C. M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).

[67] J.E. Sonier, J.H. Brewer, R.F. Kiefl, R.I. Miller, G.D. Morris, C.E. Stronach, J.S. Gardner, S.R. Dunsiger, D.A. Bonn, W.N. Hardy, R. Liang, R.H. Heffner, Science **292**, 1692 (2001); Observed static moments may also originate from charge inhomogeneities, J.E. Sonier, J.H. Brewer, R.F. Kiefl, R.H. Heffner, K. Poon, S.L. Stubbs, G.D. Morris, R.I. Miller, W.N. Hardy, R. Liang, D.A. Bonn, J.S. Gardner and N.J. Curro, cond-mat/0108479.

[68] C. Panagopoulos, B. D. Rainford, J. R. Cooper, C. A. Scott, and T. Xiang, Physica C **341-348**, 843 (2000) and cond-mat/0007158.

[69] Y. Sidis, C. Ulrich, P. Bourges, C. Bernhard, C. Niedermayer, L. P. Regnault, N. H. Andersen, and B. Keimer, Phys. Rev. Lett. **86**, 4100 (2001).

[70] B. Lake, H. M. Ronnow, N. B. Christensen, G. Aeppli, K. Lefmann, D. F. McMorrow, P. Vorderwisch, P. Smeibidl, N.Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, and T. E. Mason, Science **291**, 832 (2001).

[71] J.A. Hodges, Y. Sidis, P. Bourges, I. Mirebeau, M. Hennion, and X. Chaud, cond-mat/0107218.

[72] T. Sakai and Y. Takahashi, J. Phys. Soc. Jpn. **70**, 272 (2001) and cond-mat/0010448.

[73] W. Putikka, ITP Program on High Temperature Superconductivity (2000) and private communication.

[74] J. Schmalian, D. Pines, and B. Stojkovic, Phys. Rev. Lett. **80**, 3839 (1998).

[75] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).

[76] R. Meyer and P. Entel, Phys. Rev. B **47**, 1099 (1993).

[77] R. Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. **86**, 5377 (2001).

[78] J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989); D. Poilblanc and T. M. Rice, Phys. Rev. B **39**, 9749 (1989); H. J. Schulz, J. Physique **50**, 2833 (1989); K. Machida, Physica C **158**, 192 (1989); J. M. Tranquada, J. D. Axe, N. Ichikawa, A. R. Moodenbaugh, Y. Nakamura, and S. Uchida Phys. Rev. Lett. **78**, 338 (1997); S. A. Kivelson, E. Fradkin, and V. J. Emery, Nature **393**, 550 (1998); J. H. Han, Q. -H. Wang, D. -H. Lee, cond-mat/0006046; S. A. Kivelson, G. Aeppli, and V. J. Emery, cond-mat/0105200.